CBE 450 Chemical Reactor Fundamentals
Fall, 2011
Homework Assignment #5

1. CSTR Analysis via Numerical Analysis

Consider the following reactions

A + B → C

A + D → E

both with elementary mechanisms such that the rates are

$$r_1 = k_1 C_A C_B$$

$$r_2 = k_2 C_A C_D$$

where the rate constants are given by

$$k_1 = k_{o,1} \exp\left(-\frac{E_{a,1}}{RT}\right)$$

$$k_2 = k_{o,2} \exp\left(-\frac{E_{a,2}}{RT}\right)$$

The temperature is 300 K. The activation energy for reaction 1 is 5000 J/mol. The rate constant prefactor for reaction 1 is 0.001 liters/mole/s. The activation energy for reaction 2 is 3500 J/mol. The rate constant prefactor for reaction 2 is 0.01 liters/mole/s. The inlet flowrate is 2 liters/sec. The concentration of A in the inlet stream is 10 mol/liter. The concentration of B in the inlet stream is 10 mol/liter. The concentration of D in the inlet stream is 10 mol/liter. The reactor is initially filled with only A at 10 mol/liter.

(a) What is the steady state conversion of A for a volume of 100 liters, where conversion of A is based on the loss of A through both reactions? Show the approach to steady state of the concentrations.
(b) What volume is required to reach a 90% conversion of A at steady state, where conversion of A is based on the loss of A through both reactions?
(c) For part (b), what fraction of A was converted to C?
(d) For part (b), what fraction of A was converted to E?
(e) If you want to increase the ratio of C to E what change in operating conditions could lead to a higher yield in desired product? Use the code to illustrate this effect.

2. PFR Analysis via Analytical Expressions

Consider the following isomerization reaction

$$A \rightarrow B$$

with an elementary mechanism such that the rate is

$$r = kC_A$$

where the rate constant is given by

$$k = k_o \exp\left(-\frac{E_a}{RT}\right)$$

The temperature is 300 K. The activation energy is 5000 J/mol. The rate constant prefactor is 10.0 s^{-1}. The initial concentration of A is 10.0 mol/liter. The volumetric flowrate is 2 liter/sec.

(a) Provide an analytical expression for the reactor volume required to achieve a specified conversion for this reaction in a PFR.
(b) What length is required to reach a conversion of 95% if your PFR is a circular pipe with diameter 0.10 m?
(c) What conversion is obtained in a PFR of length 2 m, if your PFR is a circular pipe with diameter 0.10 m?

3. PFR Analysis via Numerical Analysis

Consider the reactions and rate law given in problem 1. The temperature and the inlet stream composition and flowrate are all the same as that given in problem 1.

The PFR is circular with diameter 0.10 m and length 50 m.

(a) Find the conversion of A at steady state. Show the profile of each component within the PFR.
(b) Would a CSTR of a similar volume yield a higher conversion? Why?